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The dynamic structure factor of the energy density fluctuations in the classical Heisenberg chain is studied theoretically. Using exact expressions for the first six frequency moments and the knowledge of the exact $T=0$ result, simple approximations are used to calculate the spectrum. We show rigorously that the time-dependent correlation function is different for ferro- and antiferromagnetic coupling if $T \neq 0$.

Recently, an exact expression[1,2] for the time-dependent energy-energy correlation function of the classical Heisenberg chain at $T=0$ has been obtained and an attempt to describe the energy fluctuations at nonzero temperature has been made.[1] In this paper, we extend the nonzero temperature approach of Ref. 1 by including the exact result for the sixth moment of the energy-energy correlation function and we investigate the effect of different approximations. The energy fluctuations in a Heisenberg chain in the absence of an external field are not easily probed in real experiments, but computer simulation techniques[3,4] have been used to calculate the time-dependent correlation function for short times. Therefore it is interesting to compare the qualitative features of the dynamic structure factor of Refs. 3 and 4 with the analytic approximations presented below.

The Hamiltonian of the classical Heisenberg chain is

$$H=-J\sum_i \vec{S}_i\cdot\vec{S}_{i+1} \quad , \tag{1}$$

where the $\vec{S}_i$ are classical unit vectors. In the following, we will take $J=+1$ for the ferromagnetic (FM) case and $J=-1$ for the antiferromagnetic (AFM) case. Because it is very difficult to extend the zero-temperature approach[1,2] to nonzero temperatures, we will start from the exact continued-fraction representation[5] for the normalized Laplace-transformed energy density correlation function and study the effect of different approximations. To fix the notations, we briefly recall some definitions. The normalized dynamic structure factor is given by

$$S(q,\omega)=\int_{-\infty}^{+\infty} dt e^{i\omega t}\frac{\langle E_q(t)E_{-q}(0)\rangle-\delta_{q,0}\langle E\rangle^2}{\langle E_qE_{-q}\rangle-\delta_{q,0}\langle E\rangle^2} \quad , \tag{2}$$

where E_q is the Fourier transform of the local energy

$$E_n=-J(\vec{S}_{n-1}\cdot\vec{S}_n+\vec{S}_n\cdot\vec{S}_{n+1})/2 \quad . \tag{3}$$

The dynamic structure factor can be written as[1,5]

$$S(q,\omega)=-\mathrm{Im}\cfrac{1}{z-\cfrac{\Delta_1^2}{z-\ddots\cfrac{\Delta_n^2}{z+\Sigma^{(n)}(z)}}} \quad , \quad z=\omega+i\epsilon,\ \epsilon\to 0+ \quad . \tag{4}$$

The coefficients Δ_n^2 depend on the wave vector q, the interaction J, and the temperature. The memory function $\Sigma^{(n)}(z)$ can not be evaluated exactly for nonzero temperatures and therefore we will use a relaxation time approximation[1,6]

$$\Sigma_1^{(n)}(z)=i(\Delta_{n-1}^2+\Delta_n^2)^{1/2} \quad , \tag{5}$$

and alternatively an approximation based on the assumption that $\Delta_k^2=\Delta_n^2$ for $k\geq n$

$$\Sigma_2^{(n)}(z)=-\cfrac{\Delta_n^2}{z-\cfrac{\Delta_n^2}{z-\cfrac{\Delta_n^2}{z-\ddots}}}=\frac{-z\pm(z^2-4\Delta_n^2)^{1/2}}{2} \quad . \tag{6}$$

We write $S_1^{(n)}(q,\omega)$ and $S_2^{(n)}(q,\omega)$ for the corresponding structure factors. The latter has the important property that the exact result for $T=0$ is recovered. This is easily verified by using the $T=0$ results[1]

$$\Delta_1^2=\Omega^2(q)/2 \quad , \tag{7a}$$

$$\Delta_n^2=\Omega^2(q)/4 \quad \text{for } n\geq 2 \quad , \tag{7b}$$

where

$$\Omega(q)=4|\sin q/2| \quad . \tag{7c}$$

Because of the square root in Eq. (6), $S_2^{(n)}(q,\omega)=0$ for $|\omega|>2\Delta_n$. In the present notation, the approxi-

mation of Ref. 1 is called $S_1^{(2)}(q,\omega)$.

To calculate $S_\alpha^{(n)}(q,\omega)$ $(\alpha=1,2)$ for nonzero temperature, we evaluate the frequency moments and use the expressions (3.4) of Ref. 1 together with

$$\Delta_3^2=(\langle\omega^6\rangle_q/\langle\omega^2\rangle_q-\langle\omega_q^4\rangle^2/\langle\omega^2\rangle_q^2)/\Delta_2^2 \ . \tag{8}$$

The frequency moments are defined by Eq. (3.5) of Ref. 1.

The computer program COMMUTE[7] evaluates frequency moments analytically. The exact expressions for the static structure factor, second,[8] fourth,[1] and sixth moment are given by

$$\langle E_q E_{-q}\rangle-\delta_{q,0}\langle E\rangle^2=(1-3y_1^2+2y_2)(1+\cos q)/6 \ , \tag{9a}$$

$$\langle\omega^2\rangle_q=12T^2y_1^2(1-\cos q)/(1-3y_1^2+2y_2) \ , \tag{9b}$$

$$\langle\omega^4\rangle_q=8T^2[5y_1^2+y_1^2y_2+3y_2^2-y_1^2(4+5y_2)\cos q](1-\cos q)/(1-3y_1^2+2y_2) \ , \tag{9c}$$

$$\langle\omega^6\rangle_q=8T^2(1-\cos q)(a_0+a_1\cos q+a_2\cos^2 q)/[15(1-3y_1^2+2y_2)] \ , \tag{9d}$$

where

$$a_0=448y_1^2-90y_1^3+90y_1y_2+76y_1^2y_2+180y_2^2+90y_1y_2^2-90y_1^2y_3-110y_1^2y_2^2+234y_1y_2y_3+72y_3^2 \ , \tag{9e}$$

$$a_1=-580y_1^2+135y_1^3-150y_1y_2-772y_1^2y_2-75y_1y_2^2+90y_1^2y_3-70y_1^2y_2^2-378y_1y_2y_3 \ , \tag{9f}$$

$$a_2=200y_1^2+440y_1^2y_2+260y_1^2y_2^2 \ , \tag{9g}$$

and

$$y_0=1 \ , \tag{10a}$$

$$y_1=J\left(\coth\frac{1}{T}-T\right) \ , \tag{10b}$$

$$y_n=y_{n-2}-(2n-1)JTy_{n-1} \quad \text{for } n\geq 2 \ , \tag{10c}$$

where units have been used such that $k_B=1$. The result for the sixth moment is new. In order to check the expressions (9), we use the low-temperature expansion for the y_n and we obtain

$$\langle\omega^{2n}\rangle_q=\frac{(2n-1)!!}{n!2^n}\Omega^{2n}(q) \quad \text{for } n=1,2,3 \ , \tag{11}$$

which is in perfect agreement with the exact $T=0$ result.[1] At this point, it is interesting to note that the second and the fourth moment do not depend on the sign of J while the sixth moment does. Therefore we have shown rigorously that the time-dependent energy correlation functions for the FM and AFM are not identical. This seems surprising because computer simulation data suggest that there is no difference.[4] However, for $T=0.3$ and $q=\pi/2$, the relative difference between the sixth moment of the FM and AFM is approximately 2% and very accurate simulations would be necessary to distinguish between both cases.

To investigate the effect of this difference on the dynamic structure factor, we have plotted $S_\alpha^{(n)}(q,\omega)$ for $T=0.3$ and $q=\pi/2$ and both couplings (see Figs. 1 and 2). The corresponding results of the computer simulations can be found in Ref. 3. Of course, the functions $S_\alpha^{(2)}(q,\omega)$ are the same for both figures. It is clear that the small difference in $\langle\omega^6\rangle_q$ changes the shape of $S_1^{(3)}(q,\omega)$ drastically because apart from the rightmost resonance, there is a pronounced second resonance at nonzero frequency in the AFM case.

Qualitatively the behavior of $S_2^{(3)}(q,\omega)$ is the same for both cases. Comparing the different approximations for a particular coupling we conclude that it is impossible to extract quantitative information about peak positions, intensities, or linewidths. Because at $T=0$,[1,2]

$$S(q,\omega)=[\Omega^2(q)-\omega^2]^{-1/2}\Theta(\Omega(q)-|\omega|) \tag{12}$$

consists of a continuum of modes rather than a single mode, one would expect that the spectrum at nonzero temperature is broadened substantially and this is indeed the case for $T=0.1$, $T=0.2$, and $T=0.3$ for both the FM and AFM. In several cases, we ob-

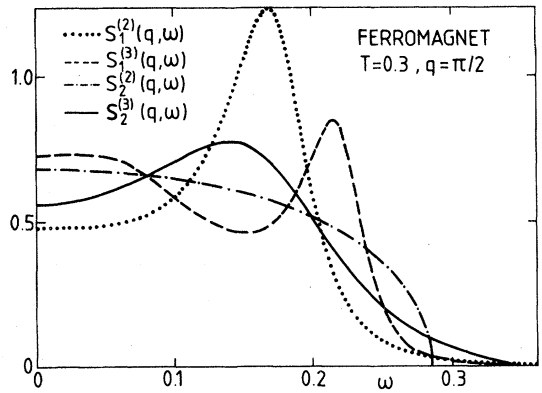

FIG. 1. The approximate dynamic structure factors of the energy fluctuations in the ferromagnet. The temperature and wave vector are the same as in Ref. 3.

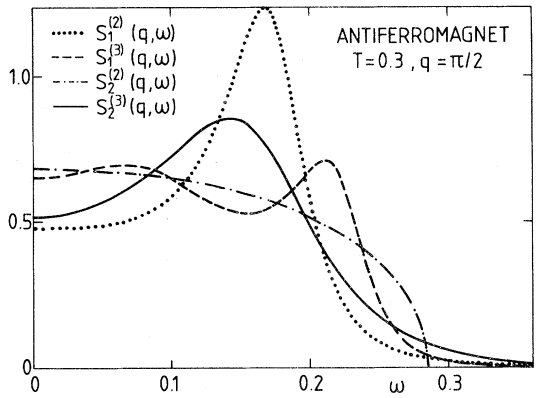

FIG. 2. The approximate dynamic structure factors of the energy fluctuations in the antiferromagnet. Note the double resonance structure in the four-pole approximation.

served additional resonances in $S_1^{(3)}(q,\omega)$ but this effect has no physical meaning because it is an artifact of the four-pole approximation.[1]

Another physical quantity of interest is the diffusion coefficient. In the hydrodynamic limit, the dynamic structure factor reduces to

$$S_\alpha^{(n)}(q,\omega) = -\mathrm{Im}(\omega + iq^2 D_\alpha^{(n)})^{-1} \ , \tag{13a}$$

where

$$D_1^{(2)} = \lim_{q\to 0} \Delta_1^2(\Delta_1^2+\Delta_2^2)^{1/2}/q^2\Delta_2^2 \ , \tag{13b}$$

$$D_2^{(2)} = \lim_{q\to 0} \Delta_1^2/q^2\Delta_2 \ , \tag{13c}$$

$$D_1^{(3)} = \lim_{q\to 0} \Delta_1^2\Delta_3^2/q^2\Delta_2^2(\Delta_2^2+\Delta_3^2)^{1/2} \ , \tag{13d}$$

and

$$D_2^{(3)} = \lim_{q\to 0} \Delta_1^2\Delta_3/q^2\Delta_2^2 \ . \tag{13e}$$

We now examine the low- and high-temperature limit of the four approximations for the diffusion coefficients. In the limit $q\to 0$, $T\to 0$, $q \ll T$ we have

$$\Delta_1^2 = 2q^2; \ \Delta_2^2 = 4T^2; \ \Delta_3^2 = 8+J \ , \tag{14a}$$

$$D_1^{(2)} = D_2^{(2)} = 1/T \ , \tag{14b}$$

and

$$D_1^{(3)} = D_2^{(3)} = (8+J)^{1/2}/2T^2 \ . \tag{14c}$$

Obviously, the temperature dependence of the diffusion coefficients at low temperatures strongly depends on the level at which the continued fraction has been truncated. In the high-temperature limit, we obtain

$$D_1^{(2)} = D_2^{(2)} = 0.8165 \ , \tag{15a}$$

$$D_1^{(3)} = 1.8161 \ , \tag{15b}$$

and

$$D_2^{(3)} = 1.9664 \ . \tag{15c}$$

These results should be compared with the computer simulation result[9] $D = 3 \pm 1$. Again, there is a large difference between the values obtained from two and three frequency moments.

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